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Three-dimensional steady state flow to a well in a randomly heterogeneous aquifer

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Abstract We consider three-dimensional steady state flow towards a well that fully penetrates a randomly heterogeneous aquifer confined between horizontal no-flow boundaries, and bounded laterally by a cylindrical, deterministically prescribed constant head boundary. The well is represented by a line sink that produces water at a deterministically prescribed constant rate Q for unit aquifer thickness. The log hydraulic conductivity, $Y = \ln K$, of the aquifer is multivariate Gaussian, statistically homogeneous with a Gaussian spatial autocorrelation function. We develop an analytical solution for the variance of hydraulic head as a function of dimensionless vertical and horizontal locations within the aquifer, variance σ_Y^2 of Y and dimensionless ratios between the principal spatial correlation scales. Our analysis is based on the non-local theory first proposed for steady state and transient flows in bounded, randomly heterogeneous media by Neuman & Orr (1993), Neuman *et al.* (1996), Guadagnini & Neuman (1999a,b) and Tartakovsky & Neuman (1998, 1999). In particular, we develop and solve analytically recursive closure approximations of the governing non-local moment equations to second order in σ_Y by means of an appropriate Green's function. We evaluate our analytical solutions by means of Gaussian quadratures for the special case of the isotropic Y field.

INTRODUCTION

It has been shown (Neuman & Orr, 1993; Neuman *et al.*, 1996; Guadagnini & Neuman, 1999a,b; Tartakovsky & Neuman, 1998, 1999) that one can render optimum unbiased predictions of hydraulic heads, $h(\mathbf{r})$, and fluxes, $\mathbf{q}(\mathbf{r})$, under ubiquitously non-uniform and uncertain field conditions by means of their ensemble (statistical) moments, $\langle h(\mathbf{r})\rangle$ and $\langle \mathbf{q}(\mathbf{r})\rangle$ respectively, generally conditioned on measurements of $K(\mathbf{r})$, $\mathbf{r}$ being location vector. The flux predictor satisfies exactly a deterministic integro-differential equation and is generally non-local and non-Darcian.

Here we consider three-dimensional steady state flow toward a well in a randomly heterogeneous domain, Ω. The boundary conditions are of constant head along the cylindrical surface or radius $r = L$ and of no-flux along the horizontal planes $z = 0, D$.

The flow domain is embedded in a multivariate Gaussian, statistically homogeneous and anisotropic log hydraulic conductivity field, $Y(\mathbf{r}) = \ln K(\mathbf{r})$.

Let $\langle K(\mathbf{r})\rangle = K_G \exp(\sigma_Y^2/2)$ be the (unconditional) ensemble mean of $K(\mathbf{r})$, representing an estimate of the random process $K(\mathbf{r})$, K_G and σ_Y being the (constant) geometric mean and standard deviation of Y, respectively; the random estimation error of $K(\mathbf{r})$ is defined as:

$$K'(\mathbf{r}) = K(\mathbf{r}) - \langle K(\mathbf{r})\rangle \tag{1}$$

In the same way we define the unconditional prediction errors of hydraulic head and flux, respectively, as:

$$h'(\mathbf{r}) = h(\mathbf{r}) - \langle h(\mathbf{r})\rangle; \qquad \mathbf{q}'(\mathbf{r}) = \mathbf{q}(\mathbf{r}) - \langle \mathbf{q}(\mathbf{r})\rangle \tag{2}$$

The hydraulic head satisfies locally the steady state continuity equation and Darcy's law:

$$-\nabla\cdot\mathbf{q}(\mathbf{r}) + f(\mathbf{r}) = 0 \qquad \mathbf{q}(\mathbf{r}) = -K(\mathbf{r})\,\nabla h(\mathbf{r}) \tag{3}$$

with the boundary conditions:

$$h(r = L, z, \theta) = H_L; \qquad \frac{\partial h}{\partial z}(r, \theta, z = 0; D) = 0 \tag{4}$$

We consider a deterministic line source $f(\mathbf{r})$ that represents a well of radius $r_w \to 0$, placed at the origin of the radial co-ordinate $r_w = 0$, given by:

$$f(r) = -\frac{Q}{2\pi r}\delta(r - r_w) \tag{5}$$

where Q is flow rate per unit aquifer thickness and δ is the Dirac delta.

Statistical averaging of equations (3) and (4), using (1) and (2), yields equations for the predictors of head and flux. Neuman & Orr (1993) have shown that the latter depend on a residual flux which is integro-differential and hence non-local and non-Darcian. To render the mean equations workable, we expand them in powers of σ_Y, following the procedure of Tartakovsky & Neuman (1998, 1999) and Guadagnini & Neuman (1999a). This nominally limits our results to mildly non-uniform fields. We note, however, that Guadagnini & Neuman (1999a,b) obtained good agreement between second order (in σ_Y) non-local moment approximations and Monte Carlo results for at least $\sigma_Y^2 = 4$ under superimposed mean uniform and convergent steady state flows in two dimensions.

Here we use non-local theory to derive analytical expressions for measures of uncertainty (variance-covariance) associated with the predictor of hydraulic head in the above three-dimensional well problem.

ANALYTICAL SOLUTION OF HEAD VARIANCE-COVARIANCE

A measure of prediction uncertainty associated with the mean head, $\langle h(r)\rangle$, is given by the head covariance, $C_h(\mathbf{r}_I, \mathbf{r}_{II}) = \langle h'(\mathbf{r}_I)\, h'(\mathbf{r}_{II})\rangle$. For a statistically homogeneous log hydraulic conductivity field ($K_G(\mathbf{r}) \equiv K_G$), to second (lowest) order of approximation, $C_h(\mathbf{r}_I, \mathbf{r}_{II})$ satisfies:

$$\nabla_{r_I} \cdot [\, K_G\, \nabla_{r_I} C_h^{(2)}(\mathbf{r}_I, \mathbf{r}_{II}) + C_{hK}^{(2)}(\mathbf{r}_I, \mathbf{r}_{II})\, \nabla_{r_I} h^{(0)}(\mathbf{r}_I)\,] = 0 \tag{6}$$

subject to boundary conditions:

$$C_h^{(2)}(\mathbf{r}_I, \mathbf{r}_{II}) = 0; \quad \text{for } r_I = L; \qquad \frac{\partial}{\partial z_I} C_h^{(2)}(\mathbf{r}_I, \mathbf{r}_{II}) = 0; \quad \text{for } z_I = 0, D \tag{7}$$

where the superscript $^{(2)}$ denotes terms that are strictly of second-order (i.e. contain only second powers of σ_Y). The solution of equations (6) and (7) is:

$$C_h^{(2)}(\mathbf{r}_I, \mathbf{r}_{II}) = \int_\Omega \nabla_{r'} C_{hK}^{(2)}(\mathbf{r}', \mathbf{r}_{II}) \cdot \nabla_{r'} h^{(0)}(\mathbf{r}')\, G(\mathbf{r}', \mathbf{r}_I)\, d\mathbf{r}' + \int_\Omega C_{hK}^{(2)}(\mathbf{r}', \mathbf{r}_{II})\, \nabla_{r'}^2 h^{(0)}(\mathbf{r}')\, G(\mathbf{r}', \mathbf{r}_I)\, d\mathbf{r}' \tag{8}$$

Here $G(\mathbf{r}, \mathbf{r}')$ is the (deterministic) Green's function of equations (6) and (7), i.e. $G(\mathbf{r}, \mathbf{r}')$ is the solution of (6) and (7) with homogeneous boundary conditions, in the presence of a point source $f(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')$; and $h^{(0)}$ is the (deterministic) zero-order approximation of the mean head, given by:

$$h^{(0)}(\mathbf{r}') = H_L + \frac{Q}{2\,\pi\, K_G} \ln \frac{r'}{L} \tag{9}$$

Substituting equation (5) in (3) and taking ensemble mean of equations (3) and (4) yields, to zero-order:

$$\nabla_{r'}^2 h^{(0)}(\mathbf{r}') = -\frac{f(\mathbf{r}')}{K_G} = \frac{Q}{2\,\pi\, K_G r'} \delta(r' - r_w) \tag{10}$$

The term $C_{hK}^{(2)}$ represents second-order approximation of the cross-covariance between hydraulic head and conductivity. It is given by (see Guadagnini & Neuman, 1999a):

$$C_{hK}^{(2)}(\mathbf{r}', \mathbf{r}_{II}) = -K_G^2 \int_{\Omega''} \nabla h^{(0)}(\mathbf{r}'') \cdot \nabla_{r''} G^{(0)}(\mathbf{r}'', \mathbf{r}_{II})\, C_Y(\mathbf{r}', \mathbf{r}'')\, d\mathbf{r}'' \tag{11}$$

where $\Omega'' \equiv \Omega$, $G^{(0)}$ is the zero-order approximation of the mean Green's function (see Guadagnini & Neuman, 1999a), and $C_Y(\mathbf{r}', \mathbf{r}'')$ is the log conductivity autocovariance. As $G^{(0)} \equiv G$, we henceforth omit the superscript $^{(0)}$. To determine $G(\mathbf{r}, \mathbf{r}')$, we first calculate the Green function for the transient problem $G(\mathbf{r}, \mathbf{r}', t)$ (Carslaw & Jaeger, 1959, p. 361–380), and then apply the property (Dagan, 1982):

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{S} \lim_{t \to \infty} \int_0^t \mathrm{G}(\mathbf{r}, \mathbf{r}', t - \tau)\, d\tau \tag{12}$$

After some developments, and upon using some properties of series containing Bessel functions (Staff of Bateman, 1953, p. 104), we obtain :

$$G(\xi, \theta, \chi, \xi', \theta', \chi') = \frac{1}{\pi\, D\, K_G} \left[\frac{1}{4} \ln \frac{1 - 2\xi\xi'\cos(\theta - \theta') + \xi^2\xi'^2}{\xi^2 - 2\xi\xi'\cos(\theta - \theta') + \xi'^2} - \sum_{m=1}^{\infty} \cos(m\pi\chi)\cos(m\pi\chi')\,\gamma_{0m} - 2\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \cos[n(\theta - \theta')]\cos(m\pi\chi)\cos(m\pi\chi')\,\gamma_{nm} \right] \tag{13}$$

where:

$$\gamma_{0m} = \begin{cases} \dfrac{I_0(\varepsilon m\pi\xi')}{I_0(\varepsilon m\pi)}\left[I_0(\varepsilon m\pi\xi)K_0(\varepsilon m\pi) - K_0(\varepsilon m\pi\xi)I_0(\varepsilon m\pi)\right] & 0 \le \xi' \le \xi \\ \dfrac{I_0(\varepsilon m\pi\xi)}{I_0(\varepsilon m\pi)}\left[I_0(\varepsilon m\pi\xi')K_0(\varepsilon m\pi) - K_0(\varepsilon m\pi\xi')I_0(\varepsilon m\pi)\right] & \xi \le \xi' \le 1 \end{cases} \tag{14}$$

$$\gamma_{nm} = \begin{cases} \dfrac{I_n(\varepsilon m\pi\xi')}{I_n(\varepsilon m\pi)}\left[I_n(\varepsilon m\pi\xi)K_n(\varepsilon m\pi) - K_n(\varepsilon m\pi\xi)I_n(\varepsilon m\pi)\right] & 0 \le \xi' \le \xi \\ \dfrac{I_n(\varepsilon m\pi\xi)}{I_n(\varepsilon m\pi)}\left[I_n(\varepsilon m\pi\xi')K_n(\varepsilon m\pi) - K_n(\varepsilon m\pi\xi')I_n(\varepsilon m\pi)\right] & \xi \le \xi' \le 1 \end{cases} \tag{15}$$

$$\xi = r/L \qquad \chi = z/D \qquad \varepsilon = L/D \tag{16}$$

and I_n, K_n are modified Bessel functions. Green's function, G, does not depend on the source term or boundary conditions, but only on boundary type (Neumann or Dirichlet) and configuration. Our reliance on G thus makes it possible for us to solve flow problems with various flow rates, Neumann conditions at the top and bottom boundaries, and Dirichlet conditions at the external cylindrical bounding surface.

Using a Gaussian anisotropic covariance for the log conductivities:

$$C_Y(\xi', \xi'', \theta', \theta'', \chi', \chi'') = \sigma_Y^2 \exp\left[-\frac{\pi}{4}\frac{L^2}{\lambda^2} d\right] \tag{17}$$

where:

$$d = \xi'^2 + \xi''^2 - 2\,\xi'\xi''\,\mathrm{Cos}(\theta' - \theta'') + \frac{e^2}{\varepsilon^2}(\chi' - \chi'')^2 \tag{18}$$

$$\lambda_x = \lambda_y = \lambda \qquad e = \lambda/\lambda_z$$

and substituting equations (9)–(18) into equation (8), we obtain the following expression for second-order approximation of the head variance $\sigma_h^{(2)} = C_h^{(2)}(\mathbf{r}_\mathrm{I} \equiv \mathbf{r}_\mathrm{II})$ in dimensionless coordinates:

$$\sigma_h^{(2)}(\xi, \theta, \chi) = \frac{Q^2 \sigma_Y^2}{4\pi^2 K_G^2}\left[\frac{L^2}{\lambda^2}\left(-2\,I_1 + \frac{1}{2\pi} I_2\right) + 4 I_3\right] \tag{19}$$

where:

$$I_1 = \int_0^1 \int_{\Omega'} \overline{G}(\xi'' = 0, \chi'', \xi, \chi)\, \overline{G}(\xi', \chi', \theta', \xi, \theta, \chi) \exp\left[-\frac{\pi}{4}\frac{L^2}{\lambda^2}\left(\xi'^2 + \frac{e^2}{\varepsilon^2}(\chi' - \chi'')^2\right)\right] \mathrm{d}\chi''\,\mathrm{d}\Omega'$$

$$I_2 = \int_{\Omega'}\int_{\Omega''} \overline{G}(\xi', \theta', \chi', \xi, \theta, \chi)\, \overline{G}(\xi'', \theta'', \chi'', \xi, \theta, \chi) \frac{\partial^2}{\partial\xi'\partial\xi''} \overline{C}_Y(\xi', \theta', \theta', \xi'', \theta'', \chi'') \frac{\mathrm{d}\Omega'\,\mathrm{d}\Omega''}{\xi'\xi''}$$

$$I_3 = \frac{1}{\sigma_Y^2} \int_0^1 \int_0^1 \overline{G}(\xi' = 0, \chi', \xi, \chi)\, \overline{G}(\xi'' = 0, \chi'', \xi, \chi)\, C_Y(\xi' = 0, \chi', \xi'' = 0, \chi'')\, \mathrm{d}\chi'\,\mathrm{d}\chi''$$

$$G = \frac{1}{\pi K_G D}\,\overline{G} \qquad \frac{\partial^2}{\partial\xi'\partial\xi''} C_Y = \sigma_Y^2 \frac{L^2}{\lambda^2}\frac{\pi}{2}\frac{\partial^2}{\partial\xi'\partial\xi''}\overline{C}_Y \tag{20}$$

To evaluate equation (19), we computed the four-dimensional integral I_1, six-dimensional I_2, and two-dimensional I_3 by Gaussian quadrature. For the cases considered, I_1 and I_3 required 20 Gauss points to yield acceptable results. The evaluation of I_2 is a formidable task. With a Pentium II 450 MHz processor (RAM is not critical), the computation of I_2 for a single point (ξ, θ, z) in the aquifer, with 14 Gauss points, takes 15 hours. Increasing the number of Gauss points from 8 to 10 improves accuracy by up to 200%, from 10 to 12 by up to 100%, and from 12 to 14 by up to 25%. We expect that a higher number of Gauss points would be needed to compute $\sigma_h^{(2)}$ with high accuracy. Nevertheless, previous numerical results by Guadagnini & Neuman (1999b) give us confidence that our results do capture key features of the general behaviour of $\sigma_h^{(2)}$.

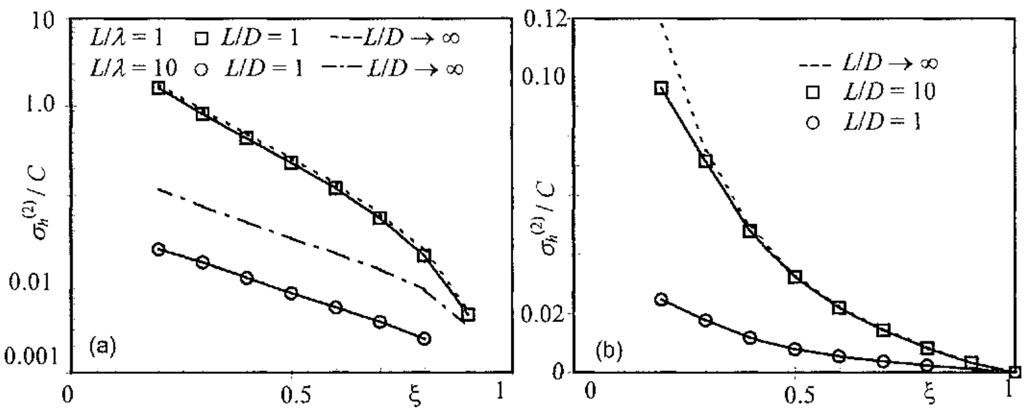

Fig. 1 Second order approximation of dimensionless hydraulic head variance as a function of ξ and (a) L/λ with $L/D = 1$, (b) L/D with $L/\lambda = 10$.

Figure 1(a) depicts the ratio $\sigma_h^{(2)}/C$ $(C = Q^2\sigma_Y^2/(4\pi^2 K_G^2))$ as a function of ξ when $\chi = 0.5$ and $\theta = 0$, for different values of L/λ, in an isotropic domain ($e = 1$) with $L/D = 1$. The head variance $\sigma_h^{(2)} \to \infty$ for $r \to r_w \to 0$, decreases as r increases, and is zero for $r = L$, due to the imposed boundary conditions. A peak head variance at the well has also been observed by Guadagnini & Neuman (1999b) in two dimensions. It is clear that $\sigma_h^{(2)}$ is strongly affected by the ratio L/λ between the characteristic scale of the flux and Y, and decreases as L/λ increases.

The head variance is also influenced by the ratio L/D between the horizontal and vertical dimensions of the domain (Fig. 1(b)). If L/D decreases, $\sigma_h^{(2)}$ decreases. Figures 1(a) and 1(b) depict $\sigma_h^{(2)}$ for the corresponding two-dimensional problem ($L/D \to \infty$); setting $D/\lambda = 1$ ($L/\lambda = 1$, $L/D = 1$; $L/\lambda = 10$, $L/D = 10$) practically reproduces the two-dimensional case.

We are currently performing further calculations to investigate the effects that vertical and angular co-ordinates, and statistical anisotropy, may have on $\sigma_h^{(2)}$.

CONCLUSIONS

Our work leads to the following major conclusions:

- Non-local stochastic theory was used to develop an analytical expression for the variance of hydraulic head in three-dimensional steady state flow towards a well that fully penetrates a randomly heterogeneous aquifer, confined between horizontal no-flow boundaries, and bounded laterally by a cylindrical, deterministically prescribed constant head boundary. The covariance is a function of dimensionless vertical and horizontal locations in the aquifer, variance σ_h^2 of Y, and dimensionless ratios between principal spatial correlation scales.
- To second order of approximation (in σ_Y), the variance $\sigma_h^{(2)}$ of hydraulic head decreases with distance from the well and as either L/λ increases or L/D decreases.

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